

## **Appendix H**

### **Operable Unit 7-13/14 Numerical Dispersion Evaluation**



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Numerical dispersion arises from the discrete finite difference approximation to continuous derivatives necessary as part of solving the governing equations for conservation of mass and momentum. The finite difference approximations use Taylor series expansions, which have multiple terms. Generally, for simplicity of coding, only the first derivative term in the expansion is used for differencing and the higher order derivative terms are neglected. Solutions obtained with this approach are only first order accurate. Finite difference approximations are used for both temporal and spatial derivatives.

Control of numerical dispersion can be accomplished by limiting the size of time steps and by increasing spatial discretization. Also, there are numerical techniques to improve representation of the derivatives. The TETRAD simulator has options available to reduce spatial numerical dispersion through use of higher order approximations of spatial derivatives. Numerical dispersion, due to time differencing, can be reduced by imposing smaller time steps, which is accomplished by specifying a lower convergence criterion.

Numerical dispersion was investigated empirically by invoking TETRAD options to control spatial dispersion, and by reducing convergence criterion to reduce the time step to control temporal dispersion. These simulations were performed for both the aquifer and the vadose zone domain. The aquifer domain results are presented first and have more detail because they could be run quickly, most simulations completing within 24 hours. The vadose zone simulation was performed using information gained from the aquifer simulations to define one simulation.

#### **H-1. AQUIFER DOMAIN NUMERICAL DISPERSION IMPACTS**

Aquifer test simulations were performed using U-238 (B\_g5), C-14 (B\_g8), and nitrate (B\_g10) to see if results from the draft RI/BRA base-case simulation were substantially impacted by numerical dispersion. Substantial would mean that results were affected such that groundwater pathway risks for that contaminant would increase past the 1.E-05 break point for deciding that the contaminant was a contaminant of concern. These contaminants were chosen to represent a range of contaminants from long-lived to nondecaying and from sorbing to nonsorbing. The aquifer simulations all used contaminant flux from the corresponding draft RI/BRA base-case vadose zone simulation without modification. The effect of dispersion in the vadose zone simulations is discussed below.

For each simulation, two methods were used to reduce numerical dispersion. The TETRAD option to use higher order differencing was used to reduce spatial dispersion. This is indicated by successively higher values of a TETRAD input parameter called “DISC”. The convergence criterion was used to reduce temporal numerical dispersion. For each simulation, impact was determined by extracting the maximum concentration as a function of time, both anywhere outside the SDA fence in the refined aquifer simulation domain and along the INL Site boundary in the base aquifer domain. Therefore, four figures are presented for each of the three contaminants in Figures H-1 through H-12.

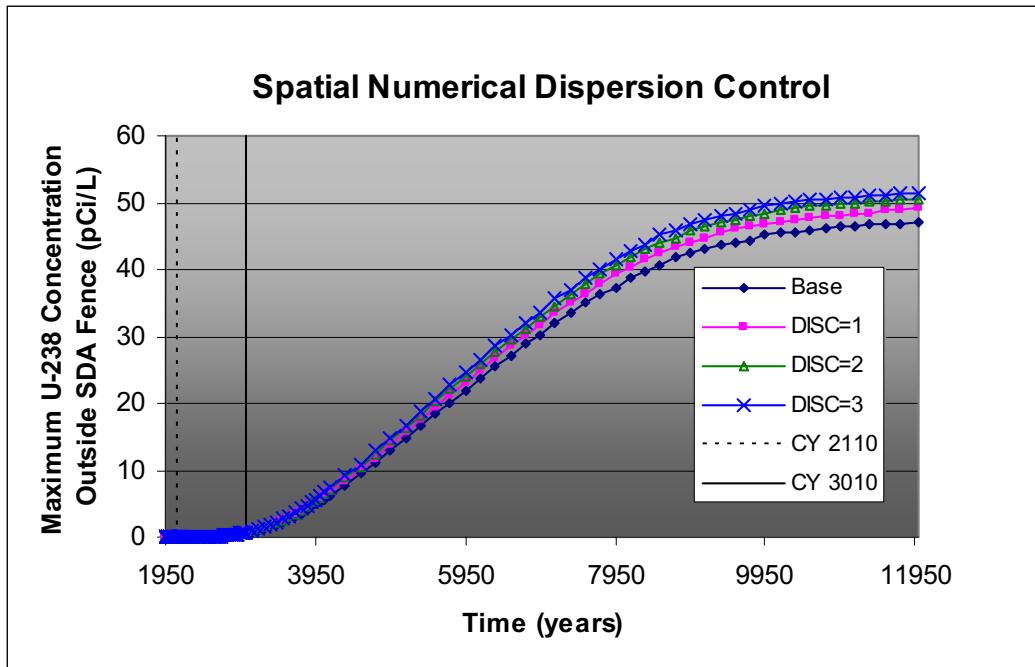


Figure H-1. Maximum simulated uranium-238 concentration outside the Subsurface Disposal Area fence with increased control of spatial numerical dispersion.

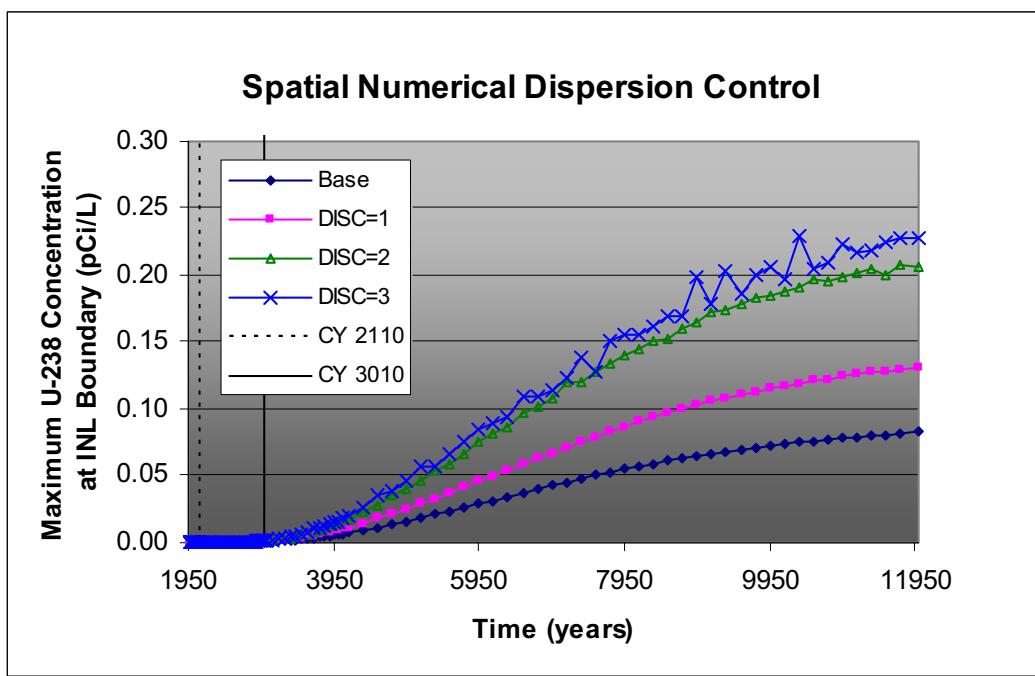


Figure H-2. Maximum simulated uranium-238 concentration along the Idaho National Laboratory Site boundary with increased control of spatial numerical dispersion.

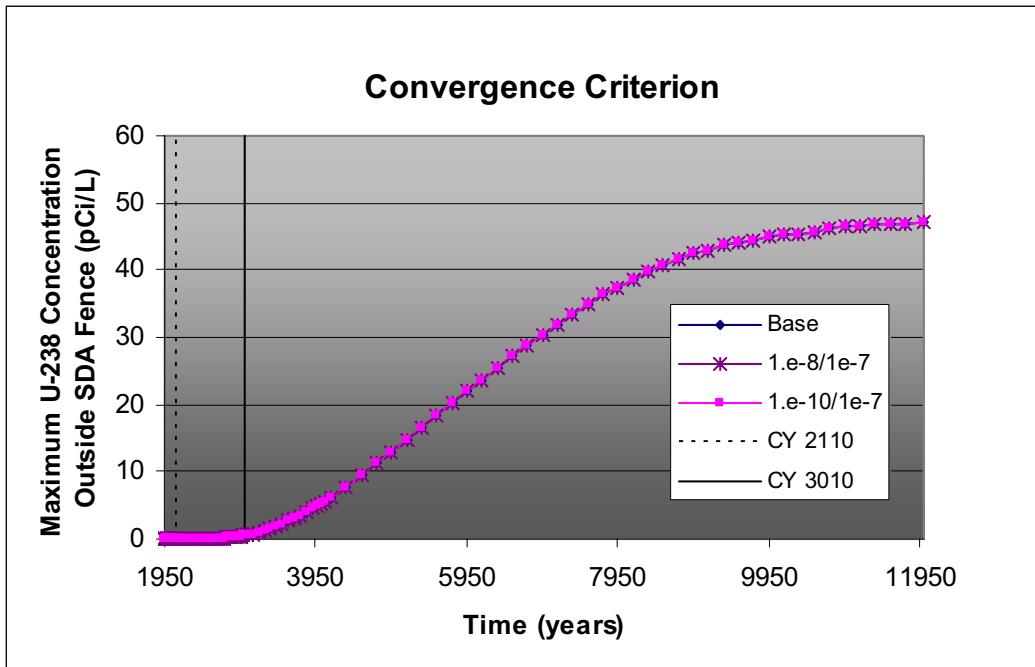


Figure H-3. Maximum simulated uranium-238 concentration outside the Subsurface Disposal Area fence with increased control of temporal numerical dispersion through smaller convergence criterion.

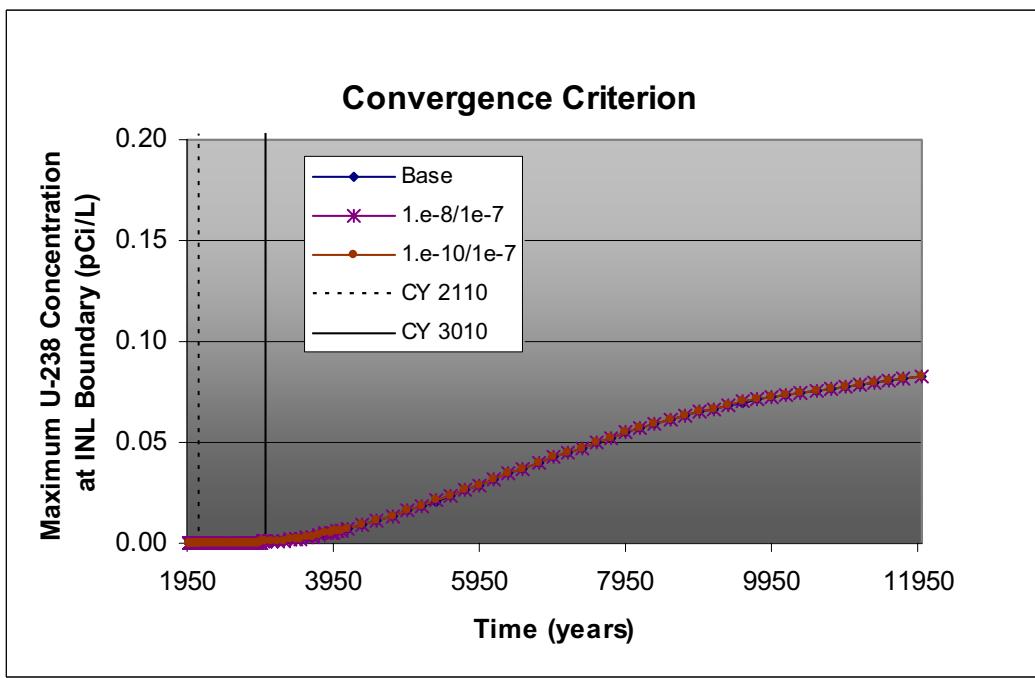


Figure H-4. Maximum simulated uranium-238 concentration along the Idaho National Laboratory Site boundary with increased control of temporal numerical dispersion through smaller convergence criterion.

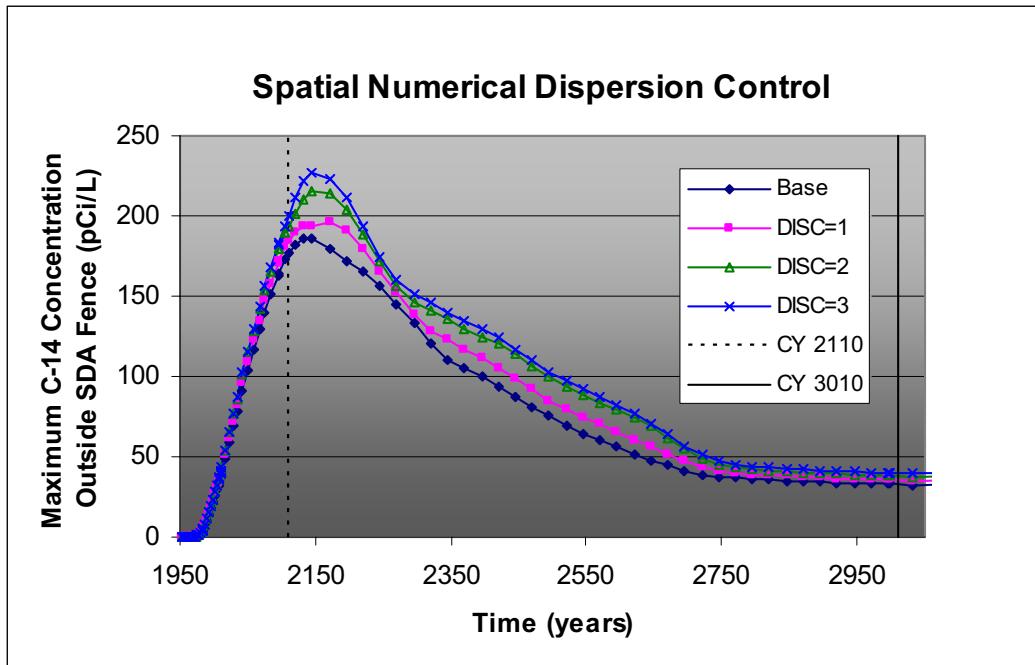


Figure H-5. Maximum simulated carbon-14 concentration outside the Subsurface Disposal Area fence with increased control of spatial numerical dispersion.

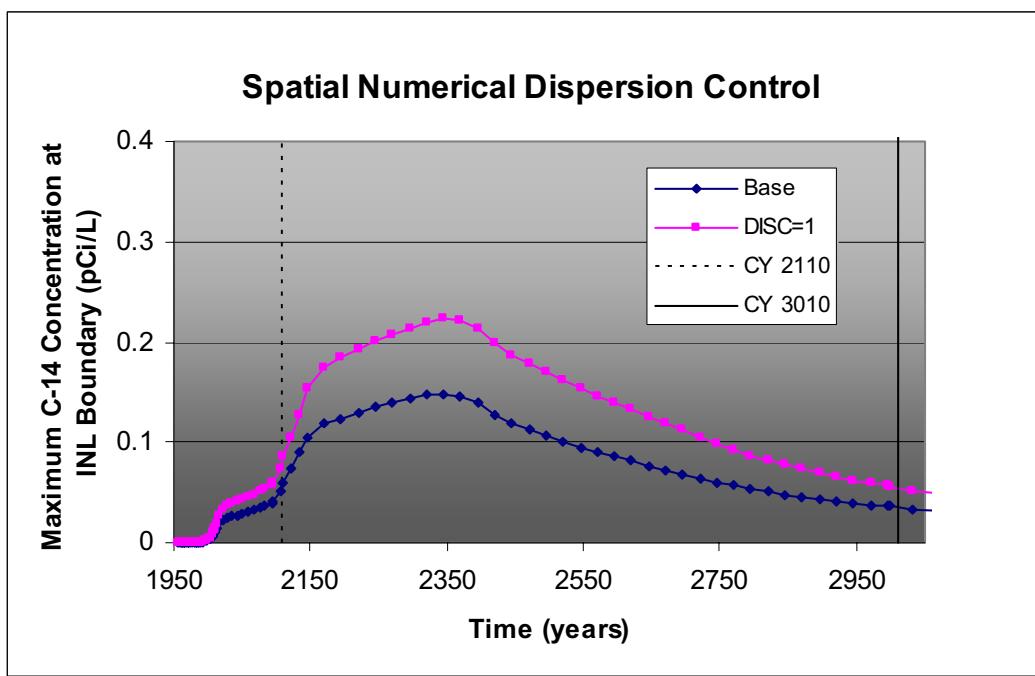


Figure H-6. Maximum simulated carbon-14 concentration along the Idaho National Laboratory Site boundary with increased control of spatial numerical dispersion.

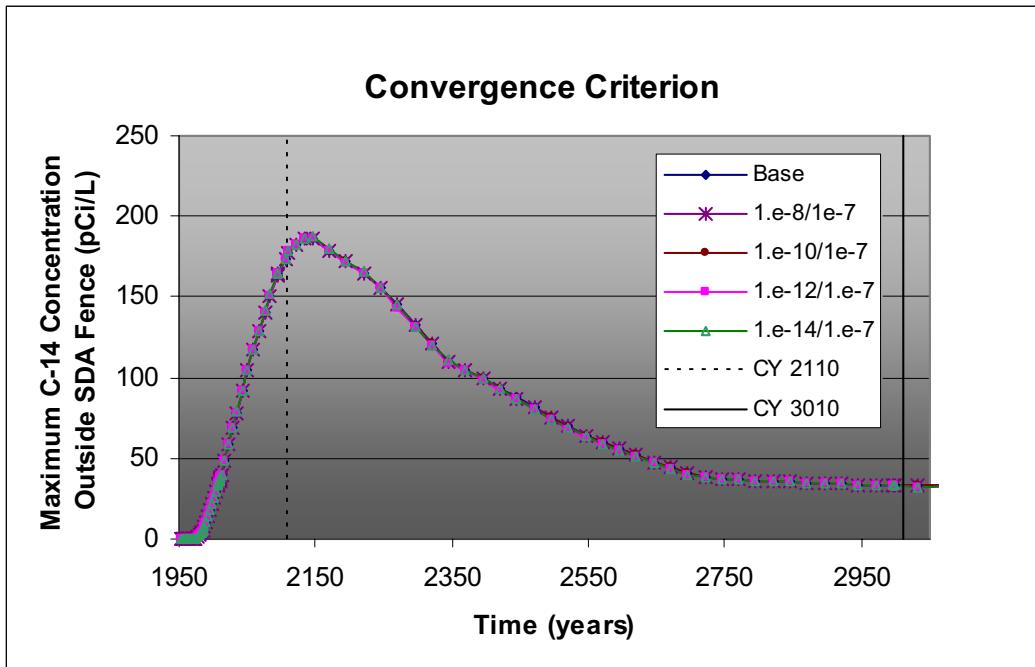


Figure H-7. Maximum simulated carbon-14 concentration outside the Subsurface Disposal Area fence with increased control of temporal numerical dispersion through smaller convergence criterion.

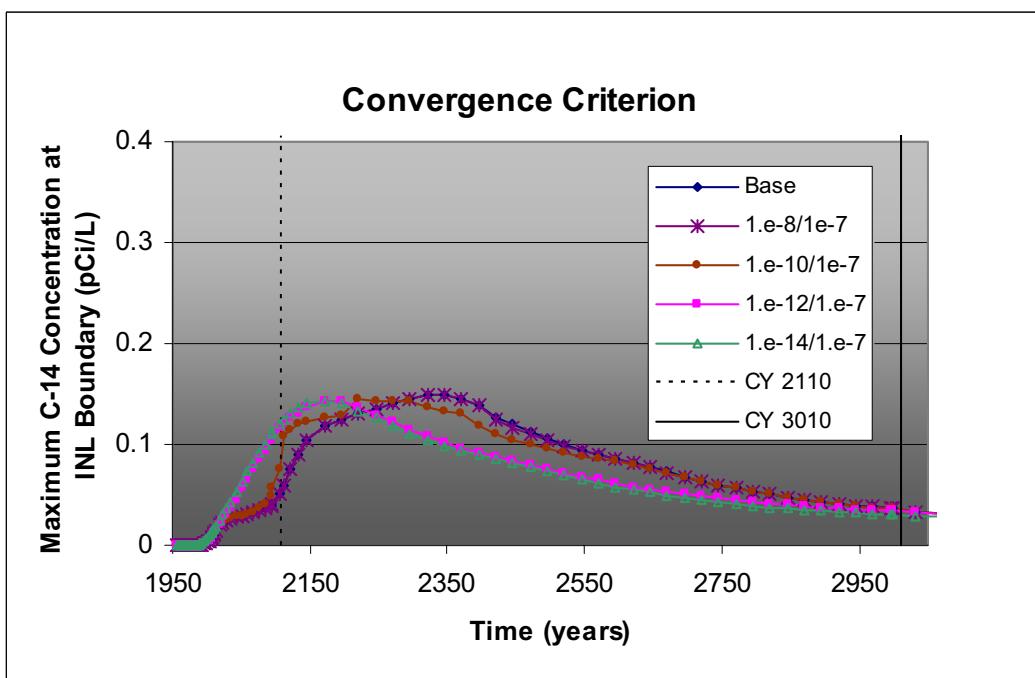


Figure H-8. Maximum simulated carbon-14 concentration along the Idaho National Laboratory Site boundary with increased control of temporal numerical dispersion through smaller convergence criterion.

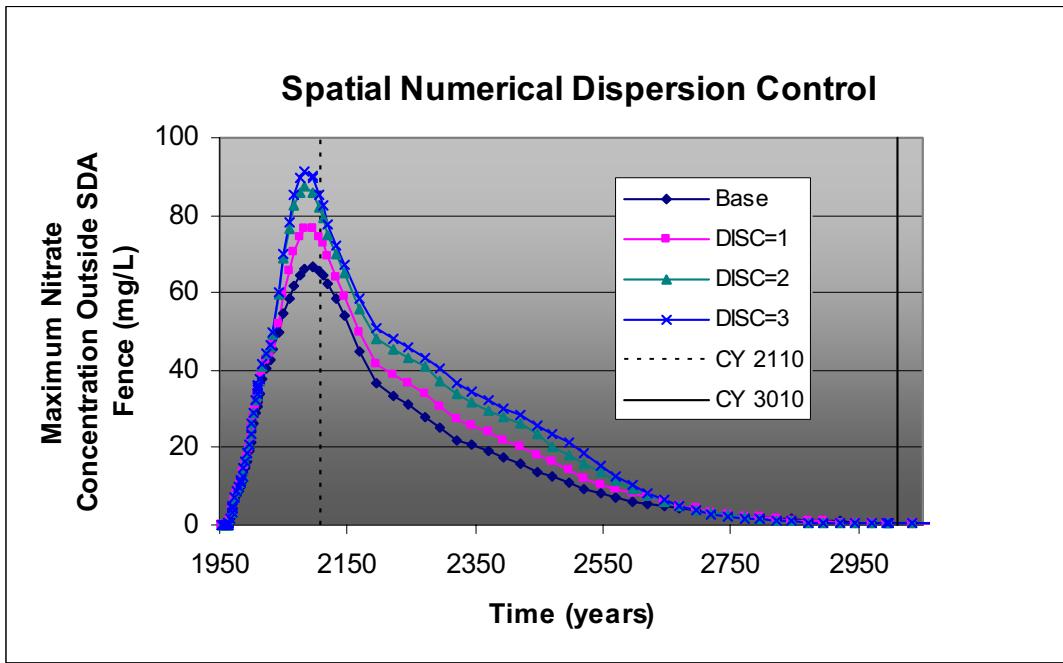


Figure H-9. Maximum simulated nitrate concentration outside the Subsurface Disposal Area fence with increased control of spatial numerical dispersion.

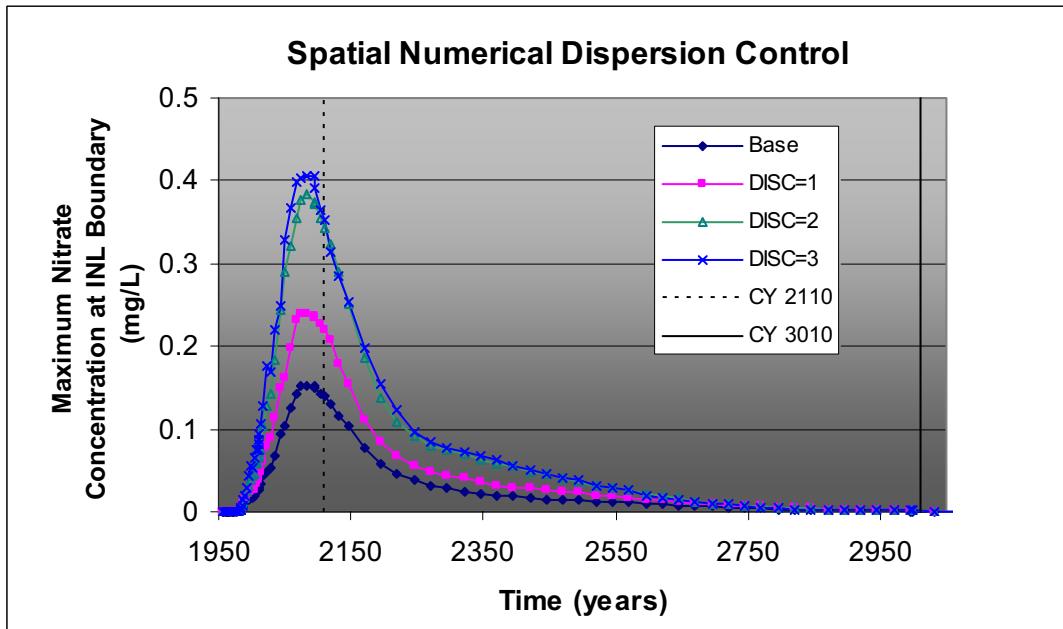


Figure H-10. Maximum simulated nitrate concentration along the Idaho National Laboratory Site boundary with increased control of spatial numerical dispersion.

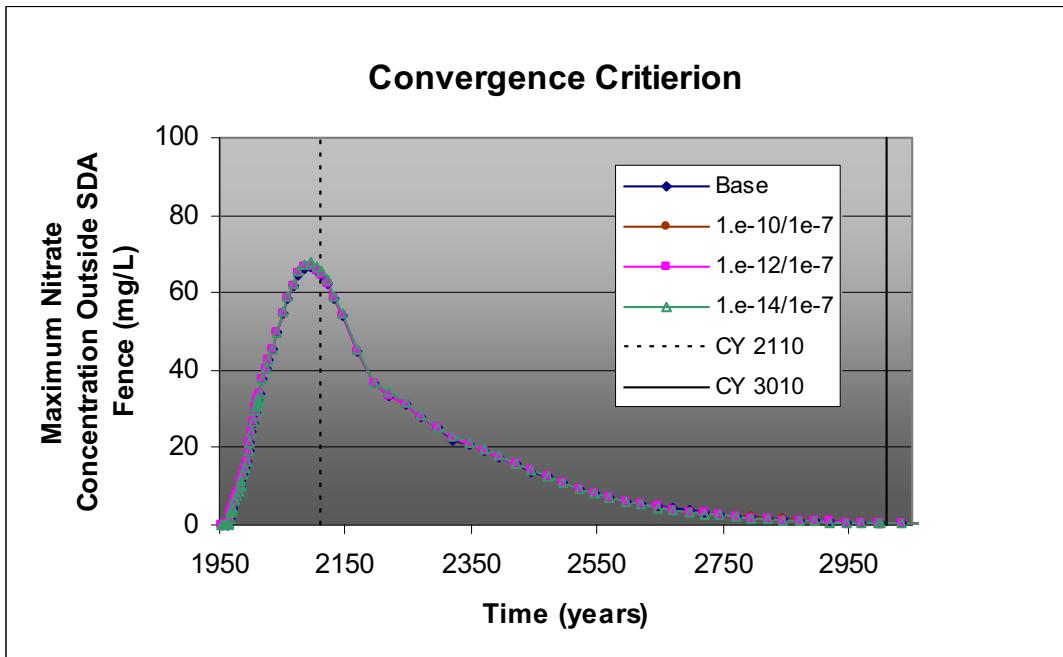


Figure H-11. Maximum simulated nitrate concentration outside the Subsurface Disposal Area fence with increased control of temporal numerical dispersion through smaller convergence criterion.

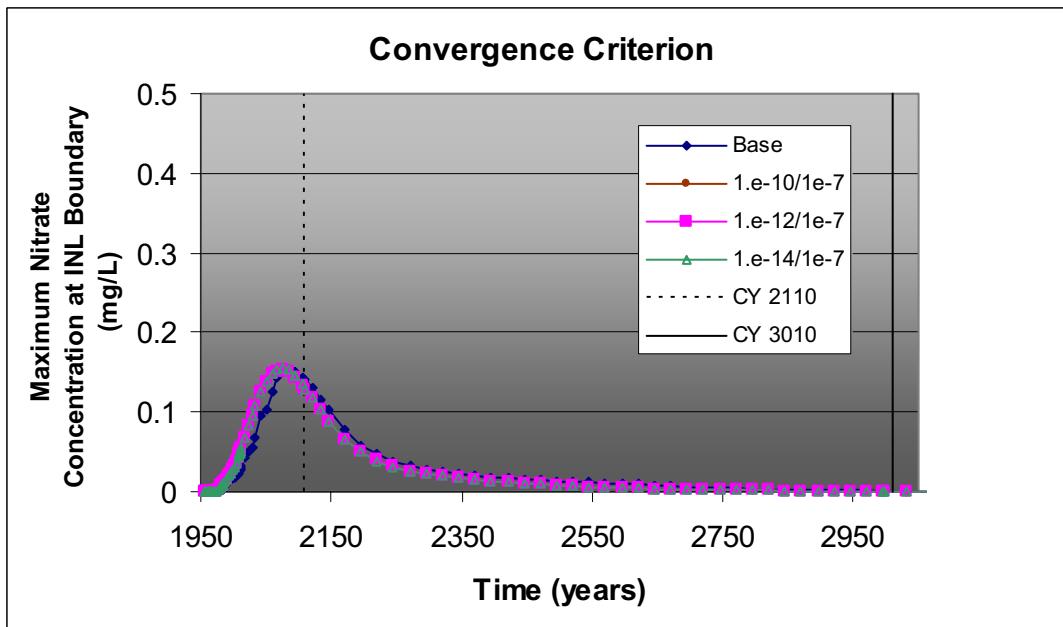


Figure H-12. Maximum simulated nitrate concentration along the Idaho National Laboratory Site boundary with increased control of temporal numerical dispersion through smaller convergence criterion.

Some observations can be made from comparing aquifer simulation results with varying levels of control on numerical dispersion. Overall, the impacts from numerical dispersion are generally small. These impacts will be evaluated quantitatively through use of scale factors. In general, impacts from spatial numerical dispersion are larger and more visible in the figures than those from temporal numerical dispersion. The impact is more apparent at the INL Site boundary than for outside the SDA fence. It is important to note that these time-history plots are for the maximum simulated concentration over time and that the location of this maximum can and does move over time. Therefore, although it appears that the total amount of mass in the system is different, the total is the same. In the C-14 simulation results, for example, the simulated maximum at any point in time with additional dispersion control is always greater than the maximum at the same point in time for the base simulation without dispersion control. As greater dispersion control is used, sometimes simulation results become unstable. This can be seen in the U-238 results at the INL Site boundary where, with the DISC parameter values of 2 and 3, the results become more variable. For the C-14 results at the INL Site boundary, the results for the DISC values of 2 and 3 are not shown because they became so unstable.

The impact from reducing convergence criterion and, therefore time step, can only be seen further away at the INL Site boundary. This was expected since the maximum concentrations extracted from the simulation results outside the SDA fence are close to the source of mass loading into the aquifer simulation, limiting the amount of numerical dispersion that could occur. Impact of the temporal numerical dispersion at the INL Site boundary location is primarily to the timing of the peak, but not to the magnitude of the peak simulated concentration.

To quantitatively assess potential impact to simulated concentrations and risks, peak values from the simulated time histories are used to create factors that can be applied to the draft RI/BRA groundwater pathway risk results to estimate the impact of numerical dispersion. These peak values were taken from simulations with improved spatial dispersion control since they yielded the largest change. Table H-1 shows peak concentrations from all simulated times and factors that would result at the two potential receptor locations, namely anywhere outside the SDA fence and along the INL Site boundary.

Table H-1. Peak concentration (pCi/L or mg/L) at receptor locations.

		U-238	C-14	Nitrate
Maximum outside Subsurface Disposal Area fence	Base	47.1	190	66.7
	With dispersion control	51.5	227	91.4
	Factor	<b>1.09</b>	<b>1.19</b>	<b>1.37</b>
Maximum along Idaho National Laboratory Site boundary	Base	0.082	0.148	0.153
	With dispersion control	0.227	0.223	0.406
	Factor	<b>2.75</b>	<b>1.51</b>	<b>2.65</b>

The maximum impact of numerical dispersion is a factor of 1.37 for outside the SDA fence and 2.75 for the INL Site boundary. To estimate impact to simulated risk, these maximum-derived factors are applied in Table H-2 to peak groundwater pathway risks for both potential receptor locations.

Table H-2. Peak 1,000-year groundwater pathway receptor risks and hazard indices for draft remedial investigation and baseline risk assessment base case and with maximum increase due to increased numerical dispersion control.

	Outside the SDA Fence Base-Case Risk	Maximum-Derived Dispersion Factor of 1.37	Along the INL Site Boundary Base-Case Risk	Maximum-Derived Dispersion Factor of 2.75
Am-241	1.E-13	2.E-13	1.E-16	4.E-16
Np-237	9.E-08	1.E-07	6.E-11	2.E-10
U-233	4.E-06	6.E-06	2.E-09	7.E-09
Th-229	3.E-07	4.E-07	1.E-10	3.E-10
Am-243	3.E-15	4.E-15	5.E-18	1.E-17
Pu-239	1.E-15	2.E-15	2.E-18	6.E-18
U-235	2.E-07	2.E-07	2.E-10	5.E-10
Pa-231	3.E-07	4.E-07	3.E-10	7.E-10
Ac-227	5.E-07	7.E-07	4.E-10	1.E-09
Pu-240	4.E-16	5.E-16	3.E-19	9.E-19
U-236	9.E-07	1.E-06	5.E-10	1.E-09
Th-232	6.E-15	8.E-15	3.E-18	8.E-18
Ra-228	4.E-14	6.E-14	2.E-17	5.E-17
Pu-238	2.E-24	2.E-24	2.E-27	6.E-27
U-234	9.E-08	1.E-07	7.E-11	2.E-10
Th-230	8.E-11	1.E-10	5.E-14	1.E-13
Ra-226	1.E-11	2.E-11	6.E-15	2.E-14
Pb-210	3.E-11	5.E-11	2.E-14	4.E-14
U-238	1.E-06	1.E-06	1.E-09	1.E-09
U-234	5.E-07	7.E-07	5.E-10	1.E-09
Th-230	5.E-10	7.E-10	3.E-13	9.E-13
Ra-226	9.E-11	1.E-10	5.E-14	1.E-13
Pb-210	2.E-10	3.E-10	1.E-13	3.E-13
Tc-99	2.E-04	3.E-04	3.E-07	9.E-07
I-129	5.E-05	7.E-05	9.E-08	3.E-07
Cl-36	1.E-06	2.E-06	2.E-09	6.E-09
C-14	1.E-05	1.E-05	8.E-09	2.E-08
Carbon tetrachloride	5.E-04	6.E-04	9.E-07	3.E-06
Methylene chloride	5.E-06	7.E-06	1.E-08	3.E-08
Nitrate	1.E+00	1.E+00	2.E-03	6.E-03
Carbon tetrachloride	1.E+01	2.E+01	2.E-02	7.E-02
Methylene chloride	3.E-02	4.E-02	5.E-05	1.E-04
Tetrachloroethylene	2.E-01	2.E-01	4.E-04	1.E-03

As can be seen from Table H-2, there are no instances of a contaminant having a peak risk in the base case that switches from below 1.E-5 to above 1.E-5. This means it is highly likely that if extensive dispersion control had been invoked all along for the aquifer simulations, there would be no difference in identification of contaminants of concern.

The impact to simulation processing time of the various dispersion control efforts was surprising. The tighter convergence controls had the expected impact of up to one order of magnitude or more increase in simulation time from the base case, which ranged from 7 hours of processing time for the C-14 simulation to 24 hours for the U-238 simulation. The impacts of invoking the higher order solution to control spatial dispersion, however, had essentially no impact on simulation time, except for the U-238 simulation, which took more than an order of magnitude longer for solutions with the TETRAD DISC parameter set to 2 or 3. In hindsight, using some improvement in dispersion control in space that would have resulted in less numerical dispersion would not have had an impact. However, since there was not a well-defined plume in the aquifer that could be definitively tied to dissolved-phase transport from the SDA, there was nothing to explicitly calibrate against and the actual dispersion is not a concern at the present time.

## **H-2. VADOSE ZONE DOMAIN NUMERICAL DISPERSION IMPACTS**

The impact of numerical dispersion in the vadose zone simulation domain was harder to assess because of the longer simulation processing times needed to run the vadose zone model. Rather than run each of the equivalent cases that were done for the aquifer model, one simulation was run with a three-order magnitude reduction in the convergence criterion (from 1.E-7 to 1.E-10) and using the TETRAD dispersion control parameter DISC set to 3. This simulation was only performed for nitrate, since it had the highest impact in the aquifer simulation for the receptor anywhere outside the SDA fence. The vadose zone flux from this simulation was input into an aquifer simulation without any dispersion control, so the impact of controlling numerical dispersion only in the vadose zone could be seen. Figure H-13 shows the comparison of the maximum simulated concentration for a receptor anywhere outside the SDA fence for the base simulation and a simulation with dispersion control. Figure H-14 likewise shows impacts on the maximum simulated concentration along the INL Site boundary.

Figures H-13 and H-14 show that the net effect on maximum simulated aquifer concentrations from reducing numerical dispersion in the vadose zone is very slight. The magnitude for the receptor location anywhere outside the SDA fence is essentially unchanged and timing is accelerated just slightly. At the INL Site boundary receptor location, the magnitude increases very slightly.

Given the very slight impacts of numerical dispersion in the vadose zone, an additional multiplicative factor to apply to the groundwater pathway risks from the draft RI/BRA was not estimated. Overall, from a perspective of both the vadose zone and aquifer simulation domains, the impact of numerical dispersion on the groundwater pathway results was minor.

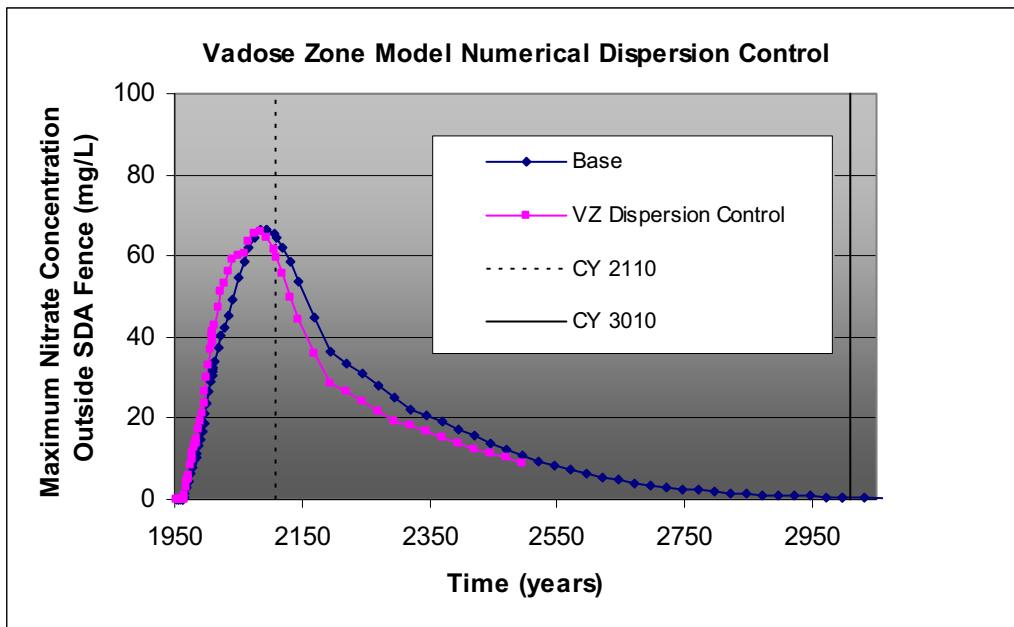


Figure H-13. Maximum simulated nitrate concentration outside the Subsurface Disposal Area fence with increased control of both spatial and temporal numerical dispersion in the vadose zone simulation.

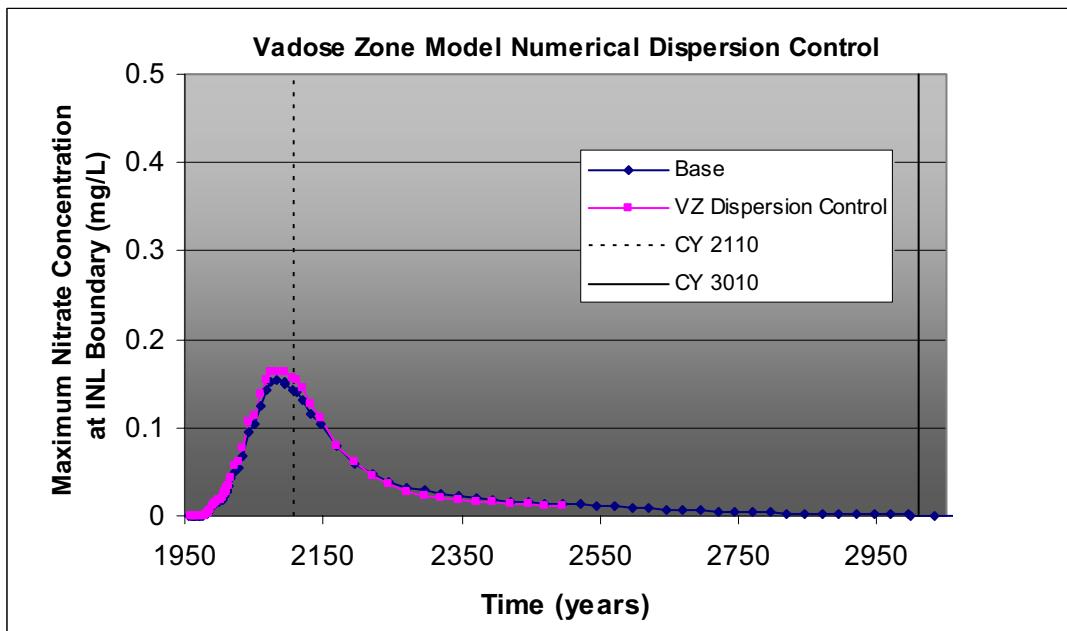


Figure H-14. Maximum simulated nitrate concentration along the Idaho National Laboratory Site boundary with increased control of temporal numerical dispersion through smaller convergence criterion.